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Effects of Electron-Interface-Phonon Interactions on Magnetopolaronic Impurity Transitions in Quantum Wells

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Effects of Electron-Interface-Phonon Interactions on Magnetopolaronic Impurity Transitions in Quantum Wells

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Electron interactions with interface phonon modes and strictly-confined bulk phonon modes are considered for the first time to calculate the magnetopolaronic effect on the transition energy of a hydrogenic impurity in the quantum well of a double heterostructure. The electron-phonon interaction is treated as a perturbation on a hydrogenic impurity confined in a quantum well under strong magnetic fields. The unperturbed states are obtained by the variational method with trial wave functions constructed on symmetry considerations. It is found that the transition energy, as a function of the applied magnetic field, breaks up into three branches with two interaction gaps occuring at two-level and three-level resonances. The lowest branch lies below the bulk TO energy. These results are found in good agreement with recent experimental data.

I. INTRODUCTION

The interface and confined bulk phonon modes in heterostructures and superlattices have been discussed theoretically[1] and observed experimentally[2] in the past. Very recently, optical phonon modes supported by a semiconductor double heterostructure (DHS) have been solved independently in the long wavelength limit by two groups.[3,4] It is found that there exist two types of phonon modes, the confined bulk modes and the interface modes. The former modes can be either longitudinal optical (LO) or transverse optical (TO) with frequencies ω_L and ω_T identical to those of the bulk excitations, while the interface (IN) modes may have frequencies between ω_T and ω_L. Eigenvectors and dispersion relations for all these modes can be found in Refs. 3 and 4. The Hamiltonian operator describing electron-optical-phonon interactions has also been derived to study the polaron mobility and magnetophonon resonance spectra,[4] and the polaronic states in a DHS.[5] The importance of interface modes are clearly demonstrated in these calculations.

subscripts

Recent experiments of far-infrared photoconductivity measurements[6] carried out for a donor impurity doped at the center of GaAs quantum wells in a GaAs/AlGaAs multiple-quantum-well (MQW) structure have revealed a surprising apparent pinning phenomenon. The resonant magnetopolaron effect on the 1s-2p+ transition energy is found to be around ω_T, in

contrast to the bulk case which has been well understood theoretically.[7] As the electron does not couple to TO phonons, the data have been regarded as a significant deviation from reasonable expectations based on the Fröhlich model of interaction with the bulk GaAs zone-center LO phonons, both in magnitude and in field dependence. The possibility of zone folding of the optical phonon dispersion has been suggested[6] to explain these results. Since all the bulk modes are strictly confined in heterostructures or superlattices, there cannot be any traveling wave in the z-direction unless the adjacent layers in the MQW structure have matching optical phonon frequencies.

We present, in this article, a detailed account of the theory, for which a brief outline has been provided.[8] The 1s-2p+ transition energy is calculated as a function of the applied magnetic field for a magnetopolaron bound to a hydrogenic impurity in the quantum well of a DHS. The electron-phonon interaction Hamiltonian derived in Refs. 4 and 5 is treated as a perturbation on the hydrogen-like impurity atom confined in a quantum well under strong magnetic fields. Since the unperturbed system cannot be solved exactly, the variational method is applied by choosing trial wave functions with proper symmetry properties. It is found that interaction gaps appear in the transition energy which then breaks into separate branches. The lowest branch lies below the TO frequency ω_T. With just one adjustable parameter in the trial wave functions, our results are already in good agreement with the newly-improved data.

Very recently, the experiment has been improved and extended in a series of measurements.[9] Both the two-level resonance (the 1s-2p+ transition energy ΔE is equal to the bulk LO phonon frequency ω_L) and the three-level resonance (ΔE is equal to $\hbar\omega_L$ plus the energy difference between levels 2p- and 1s) are observed by tuning the magnetic field. The data appear to deviate smoothly from the calculated transition energy in the absence of electron-phonon interactions, and the deviation is generally smaller than what is reported in Ref. 6. In addition, two interaction gaps corresponding to the two-level and three-level resonances are observed, and many more points are measured above the first gap. As is shown later, these data agree quite well with our theoretical curve, where possible sources of small corrections are given.

We outline the theory in Sec. II and describe the method of calculation in Sec. III. Our results are discussed along with conclusions in Sec. IV.

II. THEORY

Consider a donor impurity at the center of the GaAs quantum well of width d in a GaAs/AlGaAs DHS system. A magnetic field is applied along the growth direction. For convenience, we introduce the two-dimensional vectors $\vec{\kappa}$ and $\vec{\rho}$ such that $\vec{k} = (\vec{\kappa},q)$ and $\vec{r} = (\vec{\rho},z)$ for the phonon momentum and electron position, respectively. The electron momentum is denoted by $\vec{k}_e = (\vec{k}_{||}, k_z)$. The total Hamiltonian can be written as

$$H = H_e + H_{ph} + H_{e-ph}, \tag{1}$$

where

$$H_e = \frac{1}{2m_e}(\vec{p} - \frac{e}{c}\vec{A})^2 - \frac{e^2}{\epsilon_o r} + V_B(z) \tag{2a}$$

is the Hamiltonian for a hydrogenic impurity confined in the square well $V_B(z)$ given by

$$V_B(z) = \begin{cases} 0, & |z| \le d/2 \\ V_o, & |z| > d/2. \end{cases} \tag{2b}$$

The free phonon Hamiltonian is

$$H_{ph} = H_{LO} + H_{IN} \tag{3a}$$

$$H_{LO} = \sum_{\vec{\kappa},m} \hbar\omega_{L\nu}\left[a_m^\dagger(\vec{\kappa})a_m(\vec{\kappa}) + \frac{1}{2}\right] \tag{3b}$$

$$H_{IN} = \sum_{\vec{\kappa},j}\left\{\hbar\omega_{sj}(\vec{\kappa})\left[a_{sj}^\dagger(\vec{\kappa})a_{sj}(\vec{\kappa}) + \frac{1}{2}\right] + \hbar\omega_{aj}\left[a_{aj}^\dagger(\vec{\kappa})a_{aj}(\vec{\kappa}) + \frac{1}{2}\right]\right\}. \tag{3c}$$

In Eqs. (3), we have introduced the index ν to label the material, with $\nu = 1$ for the well and $\nu = 2$ for the barrier. We have also defined the creation (annihilation) operators $a_m^\dagger(\kappa)$ ($a_m(\kappa)$) for the confined modes and $a^\dagger_{sj,aj}(\kappa)$ ($a_{sj,aj}(\kappa)$) for the symmetric and antisymmetric interface modes of phonons. They obey the commutation relations

$$[a_\alpha(\vec{\kappa}), a_\beta^\dagger(\vec{\kappa}')] = \delta_{\alpha\beta}\delta(\vec{\kappa} - \vec{\kappa}') \tag{4a}$$

$$[a_\alpha^\dagger(\vec{\kappa}), a_\beta^\dagger(\vec{\kappa}')] = [a_\alpha(\vec{\kappa}), a_\beta(\vec{\kappa}')] = 0. \tag{4b}$$

The interaction Hamiltonian $H_{e\text{-}ph}$ is taken directly from Ref. 5. It consists of two terms: the electron interaction with confined LO modes, and the interaction with interface modes. As has been shown in Ref. 3, 5, contributions of lattice vibrations outside the well to the polaron effect are significant only when the well width d is extremely small. For $d \ge 100$ Å they are completely negligible. Therefore we have

$$H_{e-ph} = H_{e-LO} + H_{e-IN}, \tag{5a}$$

where

$$H_{e-LO} = -\sum_{\vec{\kappa}} e^{i\vec{\kappa}\cdot\vec{\rho}}\left\{\sum_{m=1,3,\cdots} B_m(\vec{\kappa})\cos(\frac{m\pi}{d}z)[a_m(\vec{\kappa}) + a_m^\dagger(\vec{\kappa})] + \sum_{m=2,4,\cdots} B_m(\vec{\kappa})\sin(\frac{m\pi}{d}z)[a_m(\vec{\kappa}) + a_m^\dagger(\vec{\kappa})]\right\} \tag{5b}$$

represents the electron interaction with confined bulk LO phonon modes in the quantum well in which q = mπ/d is quantized, and

$$H_{e-IN} = -\sum_{\vec{\kappa},j} e^{i\vec{\kappa}\cdot\vec{\rho}}\left\{B_{sj}(\vec{\kappa})\frac{\cosh(\kappa z)}{\cosh(\kappa d/2)}[a_{sj}(\vec{\kappa}) + a^{\dagger}_{sj}(-\vec{\kappa}) - B_{aj}(\vec{\kappa})\frac{\sinh(\kappa z)}{\sinh(\kappa d/2)}[a_{aj}(\vec{\kappa}) + a^{\dagger}_{aj}(-\vec{\kappa})]\right\} \quad (5c)$$

represents the electron interaction energy with interface phonon modes in the well. The normalization constants are given by

$$|B_m(\kappa)|^2 = \frac{1}{Ad}\frac{4\pi e^2\hbar\omega_{L1}}{\kappa^2 + (m\pi/d)^2}\left(\frac{1}{\epsilon_{\infty 1}} - \frac{1}{\epsilon_{01}}\right) \quad (6a)$$

$$|B_{sj}(\kappa)|^2 = \frac{\pi e^2}{A\kappa}\frac{\hbar\omega_{sj}(\vec{\kappa})}{\bar{\epsilon}_1\tanh(\kappa d/2) + \bar{\epsilon}_2} \quad (6b)$$

$$|B_{aj}(\kappa)|^2 = \frac{\pi e^2}{A\kappa}\frac{\hbar\omega_{aj}(\vec{\kappa})}{\bar{\epsilon}_1\coth(\kappa d/2) + \bar{\epsilon}_2}, \quad (6c)$$

where A stands for the interface area, $\epsilon_{\infty\nu}$ and $\epsilon_{0\nu}$ denote the optic and dielectric constants of material ν, and $\bar{\epsilon}_\nu(\omega)$ is defined by

$$\frac{1}{\bar{\epsilon}_\nu(\omega)} = \frac{1}{\epsilon_\nu(\omega) - \epsilon_{0\nu}} - \frac{1}{\epsilon_\nu(\omega) - \epsilon_{\infty\nu}}, \quad (7)$$

with the dielectric function of material ν given by

$$\epsilon_\nu(\omega) = \epsilon_{\infty\nu}(\omega^2_{L\nu} - \omega^2)/(\omega^2_{T\nu} - \omega^2). \quad (8)$$

III. METHOD OF CALCULATION

We now proceed to calculate the transition energy by perturbation theory. For the unperturbed system, we take the hydrogenic impurity in the well with a magnetic field applied normal to the interfaces. Thus $H_0 = H_e + H_{ph}$ and $H_{e\text{-}ph}$ is treated as a perturbation. The energy levels are calculated by means of Wigner-Brillouin perturbation theory to second order. The result is

$$\epsilon_i(B) = E_i(B) + \frac{1}{(2\pi)^2}\sum_n d^2\kappa\frac{|<n|H_{e-ph}|i>|^2}{\epsilon_i(B) - E_n(B) - \hbar\omega(\vec{\kappa})}, \quad (9)$$

where $E_i(B)$ stands for the corresponding unperturbed energy, and the state $|n> = |nl; N>$ is specified by the atomic state nl and the phonon number N.

It is noted, however, that even the unperturbed problem is not exactly solvable. Thus we

employ the variational method to determine the unperturbed energy levels. The trial wave function is taken to be

$$\psi = f(z)G(\rho, z, \phi). \tag{10}$$

The function f(z) in Eq. (9) is the solution to the square-well problem. It is given by

$$f(z) = \begin{cases} \cos(k_z z), & |z| \geq d/2 \\ A\exp(-k_z'|z|), & |z| > d/2 \end{cases} \tag{11}$$

where the wave numbers k_z and k_z' are related to the first electron subband energy E_1 by

$$k_z = \sqrt{2m_e E_1/\hbar^2}, \quad k_z' = \sqrt{2m_e(V_o - E_1)/\hbar^2}. \tag{12}$$

The function $G(\rho,z,\phi)$ is chosen to reflect the symmetry properties of the system. It is given by

$$G(\rho, z, \phi) = \rho^{|m|}\exp(im\phi - \gamma\rho^2/4 - \gamma\xi^2 z^2/4), \tag{13}$$

where we have defined the parameter

$$\gamma = \hbar\omega_c/2R_y, \tag{14}$$

with the cyclotron frequency $\omega_c = eB/m_e c$ and the effective Rydberg $R_y = m_e e^4/2\hbar^2$ for the impurity. The quantum number m specifies the impurity levels such that m = 1,0,-1 for the $2p_+$, 1s, $2p_-$ levels, respectively. The variational parameter ξ is determined by minimizing the energy of the level in question. All the other levels, for the particular samples used in these measurements,[9] can be neglected in these experiments. Hence the Hilbert space in our perturbation calculation is truncated to only the three states 1s, $2p_-$ and $2p_+$.

As the matrix element is generally small compared to the transition energy, the perturbation energy in (9) becomes appreciable only when the energy difference in the denominator matches the phonon energy. This implies immediately that the electron-phonon coupling has negligible influence on the 1s energy level. Hence it is sufficient to calculate $\Delta E = \varepsilon_{2p+} - E_{1s}$ for the transition energy. Furthermore, we note that significant contribution from the second term in (9) is expected around $\Delta E \approx E_{2p-} - E_{1s} + \hbar\omega$ as well as around $\Delta E \approx \hbar\omega$.

As can be seen from Eqs. (9), the calculation of energy levels involves the evaluatiuon of four matrix elements

$$\begin{aligned} M_1(\gamma) &= <2p_+, 0|H_{e-LO}|1s, 1> \\ M_2(\gamma) &= <2p_+, 0|H_{e-IN}|1s, 1> \\ M_3(\gamma) &= <2p_+, 0|H_{e-LO}|2p_-, 1> \\ M_4(\gamma) &= <2p_+, 0|H_{e-IN}|2p_-, 1>. \end{aligned} \tag{15}$$

Explicit expressions for these matrix elements are worked out in the Appendix. Here we just present the results as a function of the applied field in Fig. 1. It is observed that in both the two-level and three-level resonance cases, the interface modes always yield larger matrix elements than the corresponding confined bulk modes, and that M_4 is the largest and is generally 3 to 4 times larger than the others. This is understandable because the first Bohr radius of the impurity is of the order of the well width and the p-state wave functions extend out much farther in the xy-plane than the s-state wave function.

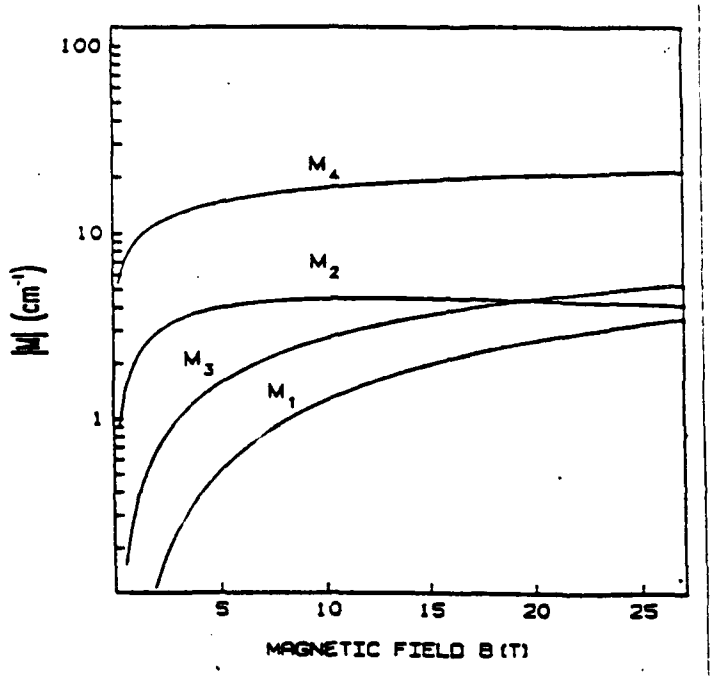

FIG. 1. Absolute value of the matrix elements of electron-phonon interactions calculated as functions of the applied magnetic field in the GaAs well of a GaAs/GaAlAs double heterostructure.

The energy of $2p_+$ level is then given by

$$\epsilon_{2p_+}(\gamma) = E_{2p_+}(\gamma) + T(\gamma), \tag{16}$$

where $T(\gamma) = T_1 + T_2 + T_3 + T_4$ represents the perturbation energy. More explicitly, we have

$$T_1 = \frac{2\alpha(\hbar\omega_L)^2}{\pi K_p d} \sum_{m=1}^{\infty} \int d^2\kappa \frac{|<2p_+|e^{i\vec{\kappa}\cdot\vec{\rho}} \sin[m\pi(\frac{z}{d}+\frac{1}{2})]|1s>|^2}{[\kappa^2 + (\frac{m\pi}{d})^2](\epsilon_{2p_+} - E_{1s} - \hbar\omega_L)}$$

$$= \frac{\alpha}{\pi}\frac{(\hbar\omega_L)^2}{K_p d} \sum_m \frac{\xi_1\xi_2 S_m^2(\gamma)}{\epsilon_{2p_+} - E_{1s} - \hbar\omega_L} \int_0^{\infty} dt \frac{t^3 e^{-t^2/\gamma}}{t^2 + (m\pi a_o/d)^2} \tag{16a}$$

$$T_2 = \frac{e^2}{4\pi\epsilon_o}\int d^2\kappa \sum_{j=1}^{2}\left\{\frac{\hbar\omega_{sj}(\kappa)}{\kappa}\frac{g_j(\kappa)}{\cosh^2(\frac{\kappa d}{2})}\frac{|<2p_+|e^{i\vec{\kappa}\cdot\vec{\rho}}\cosh(\kappa z)|1s>|^2}{\epsilon_{2p_+}-E_{1s}-\hbar\omega_{sj}(\kappa)}\right.$$
$$\left.+\frac{\hbar\omega_{aj}(\kappa)}{\kappa}\frac{g_j(\kappa)}{\sinh^2(\frac{\kappa d}{2})}\frac{|<2p_+|e^{i\vec{\kappa}\cdot\vec{\rho}}\sinh(\kappa z)|1s>|^2}{\epsilon_{2p_+}-E_{1s}-\hbar\omega_{aj}(\kappa)}\right\} \quad (16c)$$
$$= \frac{R_y}{4\pi^2}\int_0^\infty dt\frac{\xi_1\xi_2 t^2 e^{-t^2/2\gamma}}{\cosh^2(td/a_o)}\sum_{j=1}^{2}\left[\frac{\hbar\omega_{sj}(t)f_j(t,\gamma)}{\epsilon_{2p_+}-E_{1s}-\hbar\omega_{sj}(t)}\right]$$

$$T_3 = \frac{2\alpha(\hbar\omega_L)^2}{\pi K_p d}\sum_m\int d^2\kappa\frac{|<2p_+|e^{i\vec{\kappa}\cdot\vec{\rho}}\sin[m\pi(\frac{z}{d}-\frac{1}{2})]|2p_->|^2}{[\kappa^2+(\frac{m\pi}{d})^2](\epsilon_{2p_+}-E_{2p_-}-\hbar\omega_L)}$$
$$= \frac{\alpha(\hbar\omega_L)^2}{2\pi K_p d}\sum_m\frac{(\xi_2^2/\gamma)S_m^2(\gamma)}{\epsilon_{2p_+}-E_{2p_-}-\hbar\omega_L}\int_0^\infty dt\frac{t(2\gamma-t^2e^{-t^2/2\gamma})^2}{t^2+(m\pi a_o/d)^2} \quad (16b)$$

$$T_4 = \frac{e^2}{4\pi\epsilon_o}\int d^2\kappa\sum_j\left\{\frac{\hbar\omega_{sj}(\kappa)}{\kappa}\frac{g_j(\kappa)}{\cosh^2(d/2)}\frac{|<2p_+|e^{i\vec{\kappa}\cdot\vec{\rho}}\cosh(\kappa z)|2p_->|^2}{\epsilon_{2p_+}-E_{2p_-}-\hbar\omega_{sj}(\kappa)}\right.$$
$$\left.+\frac{\hbar\omega_{aj}(\kappa)}{\kappa}\frac{g_j(\kappa)}{\sinh^2(d/2)}\frac{|<2p_+|e^{i\vec{\kappa}\cdot\vec{\rho}}\sinh(\kappa z)|2p_->|^2}{\epsilon_{2p_+}-E_{2p_-}-\hbar\omega_{aj}(\kappa)}\right\} \quad (16d)$$
$$= \frac{R_y}{8\pi^2}\int_0^\infty dt\frac{\xi_2^2(2\gamma-t^2e^{-t^2/2\gamma})^2}{\gamma\cosh^2(td/a_o)}\sum_{j=1}^{2}\left[\frac{\hbar\omega_{sj}(t)f_j(t,\gamma)}{\epsilon_{2p_-}-E_{2p_-}-\hbar\omega_{sj}(t)}\right],$$

where ξ_1 and ξ_2 are the variational parameters for 1s and 2p. states, respectively, and are determined by minimizing the energy level in question, a_o is the first Bohr radius of the impurity atom, and $K_p^{-1} = (\hbar/2m_e\omega_L)^{1/2}$ measures the size of the polaron due to LO phonons. We have also defined in Eqs. (16) the variable $t = \kappa a_o$ and the functions

$$S_m(\gamma) = \int_{-d/2a_o}^{d/2a_o} dz e^{-\gamma(\xi_1^2+\xi_2^2)z^2/4}\sin\left[\frac{m\pi}{(d/a_o)}z+\frac{m\pi}{2}\right]\cos^2(k_z z) \quad (17)$$

$$f_j(t,\gamma) = g_j(t)\left[\int_{-d/2a_o}^{d/2a_o} dz e^{-\gamma(\xi_1^2+\xi_1^2)z^2/4}\cosh(tz)\cos^2(k_z z)\right]^2 \quad (18)$$

$$g_j(t) = \epsilon_{o1}/[\bar{\epsilon}_1(\omega_j)\tanh(td/2a_o)+\bar{\epsilon}_2(\omega_j)]. \quad (19)$$

The integrals in (16) are still very difficult to evaluate. We adopt a numerical iteration procedure to compute the transition energy. Let $X(\gamma) = \epsilon_{2p_+} - E_{1s}$ and $\Gamma(\gamma) = E_{2p_+} - E_{1s}$. Then Eq. (17) can be rewritten as

$$X(\gamma) = \Gamma(\gamma) + T(\gamma, X). \quad (20)$$

The function $\Gamma(\gamma)$ represents the transition energy in the absence of the electron-phonon inter-

actions and is already known from the variational calculations. Therefore, we start the iteration with $X = \Gamma(\gamma)$ in T for a fixed γ. A new X value is obtained from (20) and employed to compute a new T. The procedure goes on until self-consistency is achieved. The iteration procedure repeats when γ changes, and eventually the transition energy is found as a function of γ, which is proportional to B.

IV. RESULTS AND DISCUSSION

Results of our numerical computation are presented in Fig. 2 in which the 1s-2p+ transition energy is plotted as a function of B. The parameters used in the numerical work are d = 125 Å, $m_e = 0.067\, m_o$, $a_o = 98.7$ Å, $R_y = 5.83$ meV and $V_o = 2.30$ meV. The solid line includes the effect of the nonparabolic band mass[10] and the dashed line does not. The ~~dotted~~ line rep-

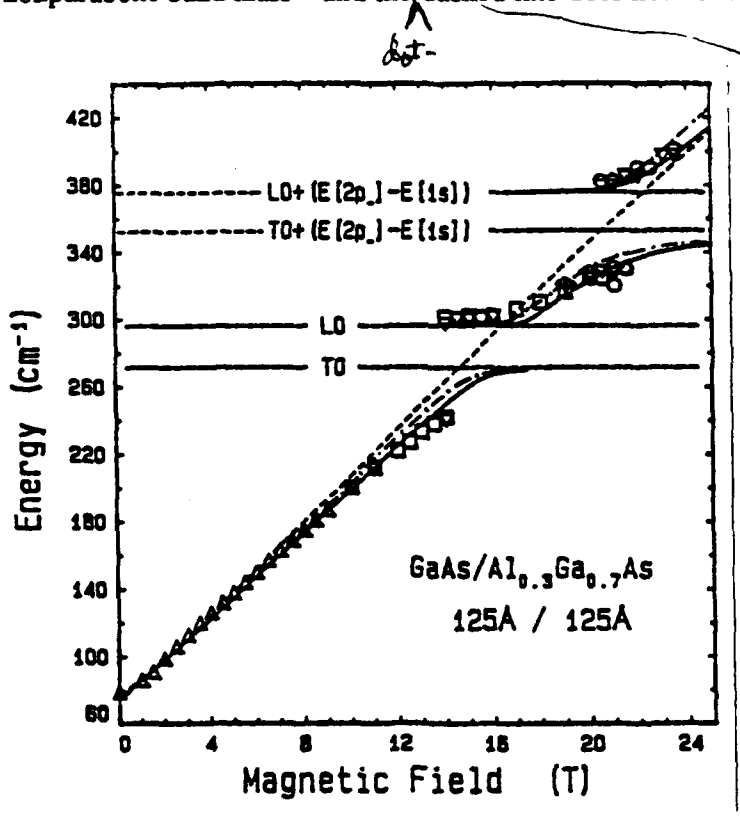

FIG. 2. Comparison of experimental data with the calculated 1s-2p+ transition energy as a function of the applied field B. The solid line represents results from the present theory including nonparablic band mass. The dashed-dotted line does not include the nonparabolicity correction, and the dashed line is the transition energy in the absence of electron-phonon interactions calculated from Greene-Bajaj wave functions with nonparabolic mass corrections included.

resents the transition energy without electron-phonon interactions. It is calculated from Greene-Bajaj wave functions[11] and corrected for the nonparabolicity effect. Experimental data are taken from a series of measurements reported in Ref. 9. It is striking that the theoretical curve breaks into three branches separated by two gaps, in good agreement with experimental data. The pinning effect, or the unperturbed energy level repelling, is apparently a result of the strong resonance interaction when the denominator of the second-order perturbation energy vanishes. As the electron does not interact with TO phonons, the appearance of the gaps can only be attributed to the coupling of the electron with interface phonons which oscillate at frequencies between the bulk ω_T and ω_L.

Further studies, both theoretical and experimental, are necessary for a complete understanding of the problem. The determination of the transition frequency from experimental data is difficult, as the observed intensity distribution in the resonance region deviates greatly from the Lorentz shape. Theoretical study of the influence of electron-phonon interactions on the transition probability is needed for detailed comparison with the experimental line shapes and observed rapid decrease in intensity in this energy region. Furthermore, as we have noted previously, the trial function (13) has only one adjustable parameter. More accurate functions must be constructed, for more accurate results.

In conclusion, we assert that it is the interaction of the electron with interface phonon modes that change the polaronic properties in the reduced geometry. These modes should always be included in the interpretation of such experiments. Since the coupling constant of the bulk Fröhlich type cannot be clearly defined for the interface modes, polaronic phenomena observed in the reduced dimensionality should never be analyzed by varying the coupling strength in terms of the bulk Fröhlich interaction.

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APPENDIX

The integration of the matrix elements can be evaluated in the following manner. We start with $M_1 = \Sigma_m M_{1m}$ where

$$M_{1m} = < 2p_+ | e^{i\vec{k}\cdot\vec{\rho}} \sin\left[m\pi\left(\frac{z}{d}+\frac{1}{2}\right)\right] | 1s > . \tag{A1}$$

Using the wave functions from Eqs. (9)-(12), we have

$$M_{1m} = c_o^2\sqrt{\frac{\gamma}{2}} S_m(\gamma) \int_0^\infty d\rho e^{-\gamma\rho^2/2}\rho^2 \int_0^{2\pi} d\phi e^{ia_o\kappa\rho\cos\phi}(\cos\phi - i\sin\phi) \tag{A2}$$

where we have defined the function

$$S_m(\gamma) = \int_{-d/2}^{d/2} dz e^{-\gamma(\xi_1^2+\xi_2^2)z^2/4} \sin\left[m\pi\left(\frac{a_o z}{d} + \frac{1}{2}\right)\right] \tag{A3}$$

As we have already noted before, the integration of z can only be done numerically. Here, we shall work on

$$\begin{aligned} I_1 &= \int_0^{2\pi} d\phi e^{ia_o\kappa\rho\cos\phi}\cos\phi \\ &= i\int_{n=0}^{\infty} \frac{(-1)^n(a_o\kappa\rho)^{2n+1}}{2(n+1)!!}\int_0^{2\pi} d\phi(\cos\phi)^{2(n+1)} \\ &= i\sum_{n=0}^{\infty}\frac{(-1)^n(a_o\kappa\rho)^{2n+1}}{(2n+1)!}\frac{[2(n+1)-1]!!}{2^{n+1}(n+1)}(2\pi) \\ &= i\pi\sum_{n=0}^{\infty}\frac{(-1)^n(a_o\kappa\rho)^{2n+1}}{2^{2n}(n+1)!n!} = 2\pi i J_1(a_o\kappa\rho) \end{aligned} \tag{A4}$$

where $J_1(a_o\kappa\rho)$ is the Bessel function. The sine term in (A2) vanishes by direct integration.

To evaluate $|M_{1m}|^2$, we need

$$\begin{aligned} &\left[\int_0^{\infty} d\rho\rho^2 e^{-\gamma\rho^2/2} J_1(a_o\kappa\rho)\right]^2 \\ &= \left[\sum_{n=0}^{\infty}\frac{(-1)^n(a_o\kappa/2)^{2n+1}}{(n+1)!n!}\int_0^{\infty} d\rho\rho^{2n+3}e^{-\gamma\rho^2/2}\right]^2 \\ &= \left[\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)!n!}\left[\frac{a_o x}{2}\right]^{n+1}\frac{1}{2}\left[\frac{\gamma}{2}\right]^{-(n+2)}\Gamma(n+2)\right]^2 \\ &= (a_o\kappa/\gamma^2)^2 e^{(-a_o\kappa)/\gamma}. \end{aligned} \tag{A5}$$

A combination of (A2), (A3) and (A5) then yields the last line of Eq. (16a).

In the calculation of M_2, we need only to consider the symmetric term, as the antisymmetric term vanishes. Thus

$$M_2 = < 2p_+|e^{i\vec{\kappa}\cdot\vec{\rho}}\cosh(\kappa z)|1s>, \tag{A6}$$

which has the same form as M_{1m} except for the z-dependence. Hence, the above procedure applies provided that $S_m(\gamma)$ is replaced by the function $f_j(t,\gamma)$ as given by (18).

The matrix element $M_3 = \Sigma M_{3m}$ where

$$
\begin{aligned}
M_{3m} &= < 2p_+ | e^{i\vec{\kappa}\cdot\vec{\rho}} \sin\left[m\pi\left(\frac{z}{d}+\frac{1}{2}\right)\right] | 2p_- > \\
&= C_1^2 S_m(\gamma) \int_0^\infty \rho^3 d\rho e^{-\gamma\rho^2/2} \int_0^{2\pi} d\phi e^{ia_o\kappa\rho\cos\phi}(\cos 2\phi - i\sin 2\phi).
\end{aligned}
\tag{A7}
$$

Again, the sine term vanishes by direct integration, and we are left with the cosine term, which is

$$
\begin{aligned}
I_3 &= \int_0^{2\pi} d\phi e^{ia_o\kappa\rho\cos\phi}\cos 2\phi \\
&= \int_0^{2\pi} d\phi \cos\phi \cos(a_o\kappa\rho\cos\phi) \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n (a_o\kappa\rho)^{2n}}{(2m)!} \int_0^{2\pi} \cos^{2n}\phi \cos 2\phi d\phi \\
&= \pi \sum_{n=0}^{\infty} \frac{(-1)^n (a_o\kappa\rho)^{2n}}{(2n)!} \frac{(2n)!!}{2^{n+1}(n+1)!} \\
&= 2\pi[1 - J_2(a_o\kappa\rho)].
\end{aligned}
\tag{A8}
$$

Substituting (A8) into (A7), we have

$$
\begin{aligned}
&2\pi \int_0^\infty \rho^3 e^{-\gamma\rho^2/2}[1 - J_2(a_o\kappa\rho)]d\rho \\
&\quad = \pi \sum_{n=0}^{\infty} \int_0^\infty \frac{(-1)^n (a_o\kappa\rho)^{2n}}{2^{2n-1}(n-1)(n+1)!} e^{-\gamma\rho^2/2}\rho^3 d\rho \\
&\quad = \pi \sum_{n=0}^{\infty} \frac{(-1)^n (a_o\kappa\rho)^{2n}}{2^{2n-1}(n-1)(n+1)!} \frac{1}{2}\left(\frac{\gamma}{2}\right)^{-(2n+4)/2}\Gamma(n+2) \\
&\quad = \pi\left[\frac{4}{\gamma} - \frac{2(a_o\kappa)^2}{\gamma^3} e^{-(a_o\kappa)^2/\gamma}\right].
\end{aligned}
\tag{A9}
$$

The evaluation of M_4 is basically the same except for a different z-dependence, and we shall not repeat it here.

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